Chapter 15

Constraints and Projection

Main concepts: Constrained dynamics, projection, first integrals via projection

15.1 Weak Invariants

In the previous sections we have looked at the case where $\nabla I(y) \cdot f(y) = 0$, so that $I(y)$ is a conserved quantity associated to any initial condition. Another case of conservation is one in which there exists an invariant submanifold $\mathcal{M}$ of dimension $d - m$ defined by $g(y) = 0$, where $g : \mathbb{R}^d \to \mathbb{R}^m$, such that if the initial condition satisfies $y_0 \in \mathcal{M}$, then $y(t) \in \mathcal{M}$ for all t.

The elements $g_i(y)$, $i = 1, \ldots, m$ are weak invariants, satisfying $\nabla g(y) \cdot f(y) = 0$ for all $y \in \mathcal{M}$ (as opposed to all $y \in \mathbb{R}^d$ for strong invariants.)

Weak invariants can be conserved by projection.

15.2 Projection

The straightforward way to obtain methods to preserve a given first integral is by projection. To motivate this, consider a vector $u \in \mathbf{R}^d$ and a linear subspace (a hyperplane P) defined by the condition

$$s \cdot y = 0$$

for some vector $s \in \mathbb{R}^d$. We can in general project u into the hyperplane by solving the following system involving a *Lagrange multiplier* λ:

$$\begin{aligned} y &= u + \lambda s, \\ 0 &= s \cdot y. \end{aligned}$$

Plugging the first equation into the second, we have

$$0 = s \cdot (u + \lambda s)$$

so that

$$\lambda = -(s \cdot s)^{-1} s \cdot u,$$

where we have assumed that s is not the zero vector so that $s \cdot s = \|s\|^2 \neq 0$. Now

$$y = u - \|s\|^{-2} s \cdot u.$$

y is called the orthogonal projection of u onto the hyperplane P.

This technique can be extended to the case where the surface of interest is not a hyperplane but instead some more general manifold of dimension R^{d-1} defined by the condition

$$I(y) = 0$$

Then, as before, we introduce a Lagrange multipler, λ and solve the (now nonlinear) equation system

$$\begin{aligned} y &= u + \lambda \nabla_y I, \\ 0 &= I(y). \end{aligned}$$

Solving this system corresponds to minimizing the functional

$$K(y) = \|y - u\|^2$$

subject to the condition $I(y) = 0$. Thus, what we are doing is finding the nearest point to u on the constraint set $\mathcal{M} = \{y | I(y) = 0\}$. It can be shown that this projection is orthogonal in the sense diagrammed in Figure 15.1a.

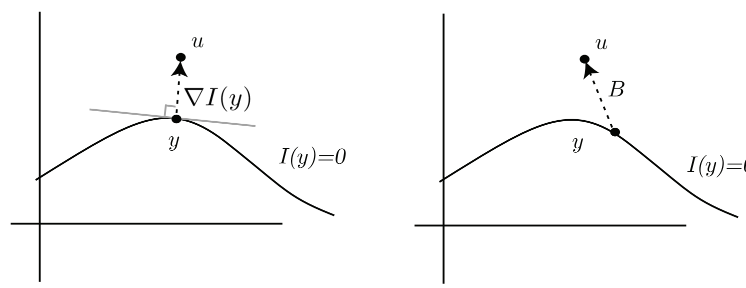

Figure 15.1: Orthogonal (a) and Oblique (b) projections onto a manifold.

There is a broader class of projections which do not necessarily find the nearest point (which is not always the essential requirement), but some other point on the constraint manifold. For example, if we know that B is *any* vector such that $s \cdot B \neq 0$, then we can solve the hyperplane projection problem by finding y and λ (which will be different than before) such that

$$\begin{aligned} y &= u + \lambda B, \\ 0 &= s \cdot y \end{aligned}$$

This type of *oblique projection* can also be of use for nonlinear manifolds. We can then use the equations

$$\begin{aligned} y &= u + \lambda B, \\ 0 &= I(y). \end{aligned}$$

(See Figure 15.1b.)

15.3 Numerical Methods with Projection

Now consider a point in space y_0 satisfying $I(y_0) = 0$. We take a step using any pth order numerical method

$$\hat{y}_1 = \Psi_h(y_0)$$

How much error can be introduced in the first integral $I(y) = 0$ by this step? Since the numerical method has local error p, we know that $\hat{y}_1$ differs from $\Phi_h(y_0)$ by at most $O(h^{p+1})$. Assuming I is a smooth function, and since we know that $I \circ \Phi_h = I$, we must have

$$I(\hat{y}_1) = I(\hat{y}_1) - I(\Phi_h(y_0)) = O(h^{p+1}).$$

The idea in *projection methods* is that we try to eliminate the small integral error by calculating the projection of the numerical solution using Ψ onto the integral manifold.

In an orthogonal projection method, we solve for y_1 so that

$$\begin{aligned} y_1 &= \hat{y}_1 + \lambda \nabla I(y_1) \\ 0 &= I(y_1) \end{aligned}$$

Here we can see already a problem: even if our original numerical method was explicit, the method obtained in this way will be implicit, since we must solve this nonlinear equation system to obtain y_1.

There is no way around solving some equations, but we can simplify our lives in many cases by using an oblique projection. The natural way to define this is to use the direction $\nabla I(\hat{y}_1)$ which is available to us after the numerical method step. Thus we think of solving for λ and y_1 from the equations

$$y_1 = \hat{y}_1 + \lambda B(\hat{y}_1) \tag{15.1}$$

$$0 = I(y_1) \tag{15.2}$$

where B is a suitable vector valued function of y. The advantage here is that we are able to compute the step by solving a single scalar nonlinear equation instead of a system of such equations (as would be the case if we used the orthogonal projection). Once y_1 is found, we use this as the starting point for the new step.

To explain, we use the example of the Lotka-Volterra model (1.6)

$$\begin{aligned} du/dt &= u(1-v) \\ dv/dt &= v(u-1) \end{aligned}$$

which has the first integral (as we know)

$$K(u,v) = \ln u + \ln v - u - v.$$

An Euler step gives $\hat{u}_{n+1}$, $\hat{v}_{n+1}$. We then may project this onto the constraint manifold $K(u,v) - K_0 = 0$ by solving

$$\begin{aligned} u_{n+1} &= \hat{u}_{n+1} - \lambda[1 - \hat{u}_{n+1}^{-1}] \\ v_{n+1} &= \hat{v}_{n+1} - \lambda[1 - \hat{v}_{n+1}^{-1}] \\ K_0 &= \ln u_{n+1} + \ln v_{n+1} - u_{n+1} - v_{n+1}. \end{aligned}$$

After introducing the first two equations into the third, we are left with a nonlinear equation to solve for λ. This could be done by Newton iteration.

Define a map Ω_h from y_n to y_{n+1} by the equations

$$\begin{aligned} \hat{y}_{n+1} &= \Psi_h(y_n) \\ y_{n+1} &= \hat{y}_{n+1} + \lambda B(\hat{y}_{n+1}) \\ I(y_{n+1}) &= 0. \end{aligned}$$

It is then a substantial exercise to analyse the conditions under which this map is well-defined and the convergence and order of accuracy of the resulting iteration scheme. However, this can be done and under mild assumptions on I and B, it can be shown that Ω_h generally retains the order of accuracy of Ψ_h.

15.4 Preserving Weak Invariants Under Discretization

We introduce the Lagrange multiplier $\lambda \in \mathbb{R}^m$ and augment (1.3)

$$\begin{aligned} y' &= f(y) + g'(y)^T \lambda \\ 0 &= g(y) \end{aligned}$$

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Let Ψ_τ be any one-step method for (1.3), and let y^*_{n+1} be the output of a single step of the method with input y_n:

$$y^*_{n+1} = \Psi_\tau y_n$$

In general $y^*_{n+1} \notin \mathcal{M}$ and so must be projected onto $\mathcal{M}$ by solving a nonlinear problem for λ:

$$g(y^*_{n+1} + g'(y^*_{n+1})^T \lambda) = 0$$

and correcting:

$$y_{n+1} = y^*_{n+1} + g'(y^*_{n+1})^T \lambda.$$

For a pth order method, the distance from y^*_{n+1} to $\mathcal{M}$ is $\mathcal{O}(\tau^{p+1})$, so convergence of Newton iteration is quite fast.

Example. Consider a particle of unit mass in an electric field $V(x)$, constrained to a sphere. The equations of motion of the free particle are:

$$\ddot{x} = -\nabla V(x)$$

The constraint is

$$g(x) = \|x\|^2 - 1 = 0.$$

The constrained equations are

$$\begin{aligned} \dot{x} &= v + 2x\lambda \\ \dot{v} &= -\nabla V(x) \\ 0 &= g(x) \end{aligned}$$

The constrained version of Euler's method is

$$\begin{aligned} x^*_{n+1} &= x_n + \tau v_n \\ v_{n+1} &= v^*_{n+1} = v_n - \tau \nabla V(x_n) \\ x_{n+1} &= x^*_{n+1} + 2x^*_{n+1}\lambda = (1+2\lambda)x^*_{n+1} \\ 0 &= g(x_{n+1}) \end{aligned}$$

where the last two equations are solved simultaneously to give λ and x_{n+1}, i.e.

$$\|x_{n+1}\|^2 = 1 = (1+2\lambda)^2 \|x^*_{n+1}\|^2 \Rightarrow \lambda = \frac{1}{2}\left(\frac{1}{\|x^*_{n+1}\|} - 1\right),$$

and x_{n+1} follows by substitution.

Remark 15.4.1 *An important point should be made regarding such projection methods: we have mentioned in the introduction to the section that a first integral is often our only way of monitoring the quality of a solution. If we design a numerical method to exactly conserve the first integral or first integrals of a system, we may destroy our only way of knowing whether the solution is correct.*